Ph.D. Synopsis submitted to

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"Studies on chemically synthesized $CuInS_2$ thin films"

For the Faculty of Science to be submitted in front of RRC

Abstract of proposed work plan/problem:

In present research work **$CuInS_2$**thin films will be deposited onto amorphous glass substrates from a mixed solution of copper chloride, indium trichloride and thiourea by simple chemical method. Structural, morphological, compositional, optical, electrical and thermo electrical properties of the deposited $CuInS_2$ thin films will be studied by using XRD, SEM, , EDAX, UV–Vis spectroscopy, DC electrical conductivity measurement and photoelectrochemical characterization technique.

1.Introduction:

The studies on thin films formation are being pursued with increasing interest on account of its proven and potential applications in variety of semiconductor devices such as solar energy photovoltaic converters. There has been considerable interest in the development of the systems for deposition of thin films which are capable of converting and storing the solar energy. Solar energy is regarded as one of the most promising renewable energies to support the sustainable development of human society. In photovoltaic cells, solar energy is converted into electrical energy. A photoelectrochemical (PEC) cell integrates capture and

conversion in one step inexpensively. Thin film solar cells are based on semiconductor thin films. For lowering the fabrication cost of solar cells different types of semiconducting materials such as CdTe/CdSe, $Cu(In_xGa_{1-x})Se_2$ (CIGS) and organic materials have been extensively studied.

Semiconductor material $CuInS_2$ has been studied as an alternative due to its optimal band gap (~1.5 eV) high absorption coefficient (~10^4 cm^{-1}). Photoelectric devices fabricated using CIS have shown efficiencies as high as **7.2%.** $CuInS_2$ semiconductor is considered to be one of the most promising materials. CIS potentially cheaper and more cost effective alternatives to CIGS family. Their band gap lies between (0.9 to 1.5 eV) has high absorption coefficients (>10^5 cm^{-1}) which are beneficial for their use in solar cell applications.

2. Review of literature and development in the subject

$CuInS_2$ belongs to the group of I-III-VI_2 compounds which are probably the most interesting ternary members in the tetrahedral family. These compounds, usually have chalcopyrite structure [1].

The group I–III–VI_2 ($CuInS_2$, $CuInSe_2$, $CuIn_xGa_{1-x}(S,Se)_2$, (CIGSSe) semiconductor materials which possess excellent optical properties with direct bang gap in the range of 1–1.5eV and high absorption coefficient of 10^4–10^5 cm-^{1} have attracted a lot of attention because of their wide range of applications, such as, electronic devices-solar cells [1–4], light emitting diode [5–9], photo catalysis [10–12], and bio-label [13,14]. Recently, with the increasingly environmental pollution and intensified energy crisis,

solarcells based on I–III–VI_2 semiconductor materials have received more and more attention [15–21]. The best power conversion efficiency of CIGS solar cells by vacuum deposited approach has exceeded 20% [22]. However, high- cost of vacuum deposited approach has greatly limited the com- mercialutilization of CIGS solar cells, it is urgent to seek a low-cost method to fabricate solar cells. Recently, the solution process to fabricate thin film solar cells has become an active research area due to its scalable utilization and low-cost.$CuInS_2$ semiconductor nano-crystals, which are one of the promising candidates in chalcopyrite family, have been investigated a lot as absorber layer material for thin film solar cells and quantum-dot sensitized solar cells. As-synthesized $CuInS_2$ chalcopyrite colloidal nanocrystals have been directly applied to fabricate Mo/CISSe/CdS/i-ZnO/ITO/Al thin film solar cells and the power conversion efficiency is achieved 5.1% [23].

3. Objectives of research/Proposed hypothesis:

Following are the objectives of present research work for the Ph.D. topic.

1) To synthesize good quality $CuInS_2$ thin films by chemical spray pyrolysis technique by optimizing various preparative parameters.

2) To characterize $CuInS_2$ thin films for physical properties like structural, morphological, compositional, optical, electrical and thermoelectrical.

3) To study photoelectrochemical solar cell performance of $CuInS_2$ thin films deposited on FTO coated glass substrates in various electrolytes.

4) To study the effect of film thickness on the properties of $CuInS_2$ thin films.

4. Methodology to be adopted:

For the preparation of $CuInS_2$ thin films one of the chemical technique will be used amongst the many more such as chemical bath deposition method, chemical spray pyrolysis, electrochemical deposition, chemical vapour deposition, vacuum evaporation and Anodization.

Chemical technique is a cheap and facile method for the preparation of quaternary chalcopyrite sulfides such as $CuInS_2$ thin films. **In this method, atomization** provides a method to get droplets of precursor with very small sizes. As the droplets approach the substrate, the solvent vaporizes, the reactant diffuse to the substrate and a heterogeneous reaction occurs, which leads to the formation of thin films. In our present work, $CuInS_2$ thin films will be prepared by chemical technique and properties of deposited films such as structural, morphological, compositional and optical characteristics characterized by XRD, SEM, EDAX,UV–Vis and electrical properties will be studied. The Photo electrochemical properties of $CuInS_2$ thin films will be studied. Also the effect of film thickness on the properties of $CuInS_2$ thin films will be studied. The work will be divided in following manner:

a) Preparation of Good Quality $CuInS_2$Thin Films.

It is proposed to grow $CuInS_2$ thin films by chemical method At initial stages the efforts will be done in order to deposit good quality $CuInS_2$ thin films on glass and FTO coated conducting glass substrates. The various preparative parameters like concentration of precursor solution, thickness, substrate temperature and other parameters will be optimized to get good quality $CuInS_2$ thin films. The as deposited films will be characterized by various characterization techniques.

b) Structural Studies:

The as deposited $CuInS_2$ thin films will be characterized by X-Ray diffraction (XRD) technique. The crystal structure, inter planar spacing, lattice planes, lattice parameters and crystallite size will be obtained and correlated with the film properties.

c) Morphological and Compositional Studies:

The morphology of the prepared $CuInS_2$ thin films will be studied by using Scanning Electron Microscopy (SEM) or Atomic Force Microscopy (AFM). The Grain Size, surface Roughness, Porosity will be studied using SEM and AFM techniques.

The Compositional Analysis of as deposited $CuInS_2$ thin films will be studied by using Energy Dispersive Analysis by X–Rays (EDAX) technique. The correlation between as taken composition and film composition will be obtained.

d) Optical Studies:

The optical absorption of $CuInS_2$ thin films will be obtained by using UV–Vis (UltraViolet–Visible) spectrophotometer. The coefficient of absorption, band gap energy (Eg), nature of transition, power factor will be obtained from optical absorption spectra.

e) Electrical and Thermoelectrical Studies:

The electrical conductivity measurements of as deposited $CuInS_2$ thin films will be carried out by using DC two point probe method. The room temperature conductivity, activation energy will be obtained and correlated with film properties. The thermoelectric power measurement studies will be carried out in order to study the type of conductivity exhibited by $CuInS_2$ thin films.

f) Photoelectrochemical Studies:

In order to find the applications of $CuInS_2$ thin films, the as deposited thin films on FTO coated conducting glass substrates will be used as active photoelectrode in Photoelectrochemical (PEC) Solar Cells. The various cell parameters of this PEC solar cells like Junction Identity Factor in Dark and under Illumination, Short Circuit Current, (Isc) Open Circuit Voltage (Voc), Fill Factor, Efficiency, Series Resistance and Shunt Resistance will be obtained.The PEC Cell will be studied for capacitance-voltage (C-V) characteristics, power output characteristics and spectral response characteristics.

g) Effect of Film Thickness:

In order to study the effect of technical parameters, the $CuInS_2$ films with different thicknesses will be obtained and studied for all above mentioned characteristics.

5. Importance of the study/Society application:

The interests of Cu-based quaternary semiconductor materials and new approaches have recently attracted increased attention for the use of low-cost thin film solar cells. $CuInS_2$ (CIS) is a semiconductor best suited for solar energy conversion because of its good chemical and mechanical stability. Photovoltaic cells fabricated using CIGS family is more costly and due to limited availability of indium and gallium such solar cells becomes expensive. Semiconductor Cu-based quaternary $CuInS_2$ (CIS) is one of the most promising materials. It is more cheap and cost effective alternatives over CIGS family.

As considering the above view, the properties of $CuInS_2$ (CIS) thin films will be studied thoroughly in the present work for societal applications like solar cells.

6. Proposed work plan/ formulation and structure of study:

Plan of work and targets to be achieved during First Year:

A through literature survey and collection of papers will be done in order to get more and deep information about work already done and scope of present work. The literature includes collection of Journals, Books and some research papers related to the present work. Various chemicals will be procured and efforts will be done

to deposit good quality $CuInS_2$ thin films. Two progress reports will be submitted at the end of this year.

Plan of work and targets to be achieved during SecondYear:

During second year, all preparative parameters will be optimized in order to get good photoactive $CuInS_2$ (CIS) thin films. All deposited films will be characterized by various techniques such as XRD, SEM, EDAX, UV–Vis, DC electrical conductivity and photoelectrochemical technique. Also we will try to submit two or more research papers to reputed international research journals. Two progress reports will be submitted at the end of this year.

Plan of work and targets to be achieved during Third Year:

Results obtained in second year will be analyzed and published in reputed journals. Also the outcomes of our research work will be presented in national and international gatherings such as Seminars, Workshops, and Conferences during this year. Once this is done final synopsis will be submitted and after this thesis will be written. Thesis will be submitted to the university.

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